Phase separation in the neutral Falicov-Kimball model

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Abstract

The Falicov-Kimball model consists of spinless electrons and classical particles (ions) on a lattice. The electrons hop between nearest neighbor sites while the ions do not. We consider the model with equal numbers of ions and electrons and with a large on-site attractive force between ions and electrons. For densities 1/4 and 1/5 the ion configuration in the ground state had been proved to be periodic. We prove that for density 2/9 it is periodic as well. However, for densities between 1/4 and 1/5 other than 2/9 we prove that the ion configuration in the ground state is not periodic. Instead there is phase separation. For densities in $(1/5, 2/9)$ the ground state ion configuration is a mixture of the density 1/5 and 2/9 ground state ion configurations. For the interval $(2/9, 1/4)$ it is a mixture of the density 2/9 and 1/4 ground states.

1 Introduction

The spinless Falicov-Kimball model has two types of particles: spinless electrons and classical particles, which we refer to as ions. The particles are on a lattice with the restriction that there is at most one ion at each lattice site. The spinless electrons are fermions, so there is at most one electron per site. The electrons can hop between nearest neighbor sites, but the ions cannot. There is an on-site interaction between electrons and ions. The Hamiltonian is

$$H = \sum_{<x,y>} c_x^\dagger c_y - 4U \sum_x c_x^\dagger c_x V_x \tag{1}$$

where $c_x^\dagger$ and c_x are creation and annihilation operators for the electrons. V_x is the occupation number for the ions, i.e., $V_x = 1$ if there is a ion at x and $V_x = 0$ if there is not. The sum over $< x, y >$ is over nearest neighbor bonds in the lattice. (The factor of 4 in front of the U is included for latter convenience.) This paper is only concerned with the square lattice, although the model may be defined on any lattice. We will only consider the neutral model in which the number of electrons is equal to the number of ions, and the interaction parameter U will be large and positive. By a hole-particle transformation results for positive U imply results for negative U, but we will not bother to state them.

A review of rigorous work on the Falicov-Kimball model may be found in [4]. Here we mention only some of the work on the neutral model for large positive U. In one dimension it is expected that for large U the ground state of the neutral model with rational density is the periodic arrangement of the ions which is "most homogeneous." (There is an explicit algorithm for determining the most homogeneous configuration.) This was proved by Lemberger for $U > U_c$ where U_c depends on the denominator of the rational density [7]. In any number of dimensions the ground state for density 1/2 is the checkerboard configuration for all $U > 0$ [1, 6]. In two dimensions with large U the ground states for densities $1/3, 1/4$ and $1/5$ are known rigorously and are periodic [3, 5]. For densities between 1/4 and 1/2 there are partial results on the ground state [5], but there is no proof it is periodic for rational densities. Based on what is known in one and two dimensions and the methods used to obtain these results, it is natural to conjecture that in two dimensions the ground state for large U is periodic for rational densities.

In this paper we prove that this conjecture is wrong for densities between 1/5 and 1/4 other than 2/9. In this density range there is phase separation in the ground state. The phases involved are the ground states for densities 1/5, 2/9 and 1/4, which are shown in figure 1 . The ground state for densities between 1/5 and 2/9 is made up of large regions of density 1/5 and density 2/9 ground states with the relative areas chosen to yield the desired density. A similar statement holds for densities between 2/9 and 1/4. The precise theorem is as follows.

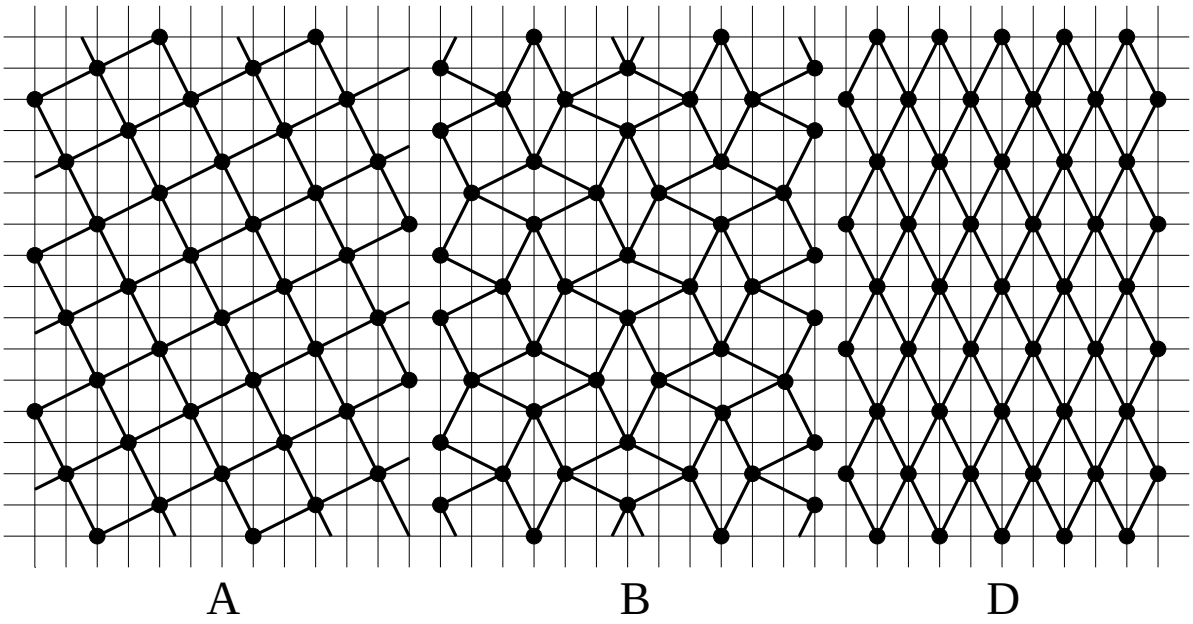

Figure 1 : The ground states for densities 1/5, 2/9 and 1/4 (left to right). The heavy lines between the ions are only a guide for the eye.

Theorem 1 *There are positive constants U_0 and c such that for $U \geq U_0$ the following is true for L by L squares Λ with n ions and n electrons. Let $\rho = n/L^2$ be the common density. If the density ρ is $2/9$, L is a multiple of 6 and we use periodic boundary conditions, then the ground state configurations of the ions are configuration B in figure 1 and its translates. If the density ρ is between $1/5$ and $2/9$, then for every ground state configuration of the ions we can find a subset Λ_0 of Λ which contains at most cU^8L sites and is such that on each connected component of $\Lambda \setminus \Lambda_0$ the configuration agrees with either configuration A or B in figure 1 (up to a lattice symmetry). If the density ρ is between $2/9$ and $1/4$, then the same statement is true with "A or B" replaced by "B or D." (The statements for densities other than $2/9$ are true for any choice of boundary conditions.)*

Although U^8 is large, the key point is that the bound on the number of sites in Λ_0 contains L while the number of sites in Λ is L^2. So for large L, Λ_0 is a tiny fraction of the total area. We can think of Λ_0 as consisting of domain walls between large regions which contain one of the configurations shown in figure 1. The phase separation we find in this range of densities for the neutral model should not be confused with the phase separation discussed by Freericks and Falicov [2]. Their argument applied to the non-neutral model.

The expectation that the neutral model with rational density should have periodic ground states is based on the following intuition. The attraction between electrons and ions is large, so each electron spends most of its time at a site with an ion. Now consider

the kinetic energy of an electron. If nearby sites have ions, then the electrons at those sites will restrict the movement of the electron we are considering. So its kinetic energy is minimized by spreading out the ions as much as possible to maximize the space that each electron has to move in. However, Watson [8] emphasized that there will typically be a mismatch between the lattice and the natural ion configuration in the absence of a lattice. Thus the lattice structure can frustrate the exclusion principle's attempts to put the ions in the "most homogeneous" configuration. We should emphasize that this paper only covers a small interval of densities. An important open question is whether the phase separation we find here holds for most densities, or whether there are intervals in which the rational densities have periodic ground states which are the most homogeneous in some sense.

We conclude the introduction by sketching the proof for densities in $(1/5, 2/9)$. When U is large and the model is neutral, the ground state energy of a given ion configuration may be expanded in powers of $1/U$. This yields an effective Hamiltonian for the ions. One can begin to study it by only keeping terms up to a certain order in $1/U$. (Of course, to prove anything one must eventually consider all orders.) Watson [8] showed that when the density is between 1/5 and 1/4 the ground states of the fourth order Hamiltonian correspond to tilings of the plane by squares and diamonds in which the squares and diamonds have the dimensions of those found in figure 1 . Watson's result will play a crucial role in our proof. The vertices in such a tiling can be one of four types which we label A, B, C or D following Watson's notation. The four types are shown in figure 3 . Note that in figure 1 configurations A, B or D contain only vertices of type A, B or D, respectively.

All configurations that correspond to a square-diamond tiling have the same energy through fourth order. To determine the ground states for densities in $(1/5, 2/9)$ we must go to higher orders in the perturbation series. Following Watson's treatment of a similar model, we write the Hamiltonian as a function of the number of each type of vertex. At sixth order these square-diamond tilings still all have the same energy. At eighth order vertices of type A,B and C have the same energy but vertices of type D have higher energy. For densities between 1/5 and 2/9 there are square-diamond tilings which contain no vertices of type D. To determine the ground state among all these configurations we must go to tenth order. Here we find that the energy of a type C vertex is higher than that of a type B vertex. Thus for densities in $(1/5, 2/9)$ the ground state must be a square-diamond tiling with only type A and B vertices. (Note that the tiling with only type A vertices has density 1/5, while the tiling with only type B vertices has density 2/9. So one can obtain any density in $(1/5, 2/9)$ by a suitable mix of type A and B vertices.) However, a type A vertex cannot be adjacent to a type B vertex. Thus we must separate the A and B vertices to minimize the energy.

2 Proof of phase separation

To derive the perturbation theory it is convenient to change to "spin" variables for the ions. Let $2V_x = S_x + 1$, so $S_x = 1$ when there is an ion at x and $S_x = -1$ when there is not. We then take

$$H = \sum_{<x,y>} c_x^\dagger c_y - 2U \sum_x c_x^\dagger c_x S_x$$

This differs from the original Hamiltonian by a term proportional to $\sum_x c_x^\dagger c_x$, but we will only consider problems in which the number of electrons is fixed, so such a term is constant.

There are no interactions between the electrons, so the Hamiltonian is just the second quantized form of the single electron Hamiltonian $T - 2US$. The operator T has matrix elements T_{xy} with $T_{xy} = 1$ if $|x - y| = 1$ and $T_{xy} = 0$ otherwise. The operator S is diagonal with entries S_x. The ground state energy for N electrons is the sum of the N lowest eigenvalues of $T - 2US$. To find the ground state for a particular density of electrons and ions we must minimize this energy over all S with the desired ion density.

Let $H(S)$ be the ground state energy for the ion configuration S with the number of electrons equal to the number of ions. To expand $H(S)$ in powers of $1/U$, we begin by rewriting $H(S)$ as in [6]. If $U > 2$ then the number of negative eigenvalues of $T - 2US$ is equal to the number of sites with $S_x = 1$, i.e., the number of ions. Thus when the number of electrons equals the number of ions, we have

$$H(S) = \sum_{\lambda_i < 0} \lambda_i = \frac{1}{2}[Tr(T - 2US) - Tr(|T - 2US|)] \tag{1}$$

where λ_i are the eigenvalues of $T-2US$. Now $Tr(T) = 0$, and if we keep the number of ions fixed then $Tr(S)$ is a constant. So we might as well redefine $H(S) = -\frac{1}{2}Tr(|T - 2US|)$. Then we write this as

$$H(S) = -\frac{1}{2}Tr(|T - 2US|) = -\frac{1}{2}Tr([(T - 2US)^2]^{\frac{1}{2}}) = -UTr(1 + \Delta)^{\frac{1}{2}} \tag{2}$$

with

$$\Delta = -(2U)^{-1}(TS + ST) + (2U)^{-2}T^2$$

We have used the fact that $S^2 = 1$.

Now we derive the perturbation theory by following the treatment by Gruber, Jedrzejewski and Lemberger [3]. A somewhat different derivation may be found in [7]. If U is sufficiently large, then $||\Delta|| < 1$ and we may expand $(1 + \Delta)^{\frac{1}{2}}$ in a power series in Δ. Since T_{xy} is nonzero only if x and y are nearest neighbors, when we take the trace of each term we generate nearest neighbor walks that end where they start. Grouping together terms with the same power of U^{-1}, we may write the result as

$$H(S) = \sum_{m=1}^{\infty} U^{-2m+1} \sum_X h_{2m,X} S_X \tag{3}$$

X is summed over finite subsets of the lattice, and $S_X = \prod_{x \in X} S_x$. The coefficient $h_{2m,X}$ is nonzero only if there is a nearest neighbor walk with $2m$ steps which ends where it begins and visits each site in X. (It may visit sites outside of X as well.) The coefficients $h_{2m,X}$ are invariant under the usual lattice symmetries. There is a constant c such that for every site x

$$\sum_{X: x \in X} |h_{2m,X}| \leq c^m \tag{4}$$

We need to compute this effective Hamiltonian through tenth order, i.e., through the $m = 5$ terms. There are a lot of terms at this order. Since we will consider relatively low densities, it will prove useful to go back to the occupation variables V_x. (Recall that $S_x = 2V_x - 1$.) Equation (3) gives

$$H(V) = \sum_{m=1}^{\infty} U^{-2m+1} \sum_X c_{2m,X} V_X \tag{5}$$

where $V_X = \prod_{x \in X} V_x$. The coefficients $c_{2m,X}$ may be computed from the $h_{2m,X}$ in a straightforward manner. In particular, they are nonzero only if X is contained in the set of sites visited by a $2m$ step nearest neighbor walk that ends where it begins. The $c_{2m,X}$ satisfy a bound like (4).

For the proof it is useful to split the effective Hamiltonian into three parts.

$$H = H_4 + H_{10} + H_\infty \tag{6}$$

H_4 contains the terms in eq. (5) for $m = 1$ and 2. H_{10} contains the terms with $m = 3, 4$ and 5, and H_∞ contains the terms with $m > 5$. The fourth order Hamiltonian H_4 has been computed before [3]. In the occupation variables it may be written in the following form.

$$\begin{aligned} H_4 = \quad & U^{-1}[8 \sum_{<xy>:|x-y|=1} V_x V_y - 16 \sum_x V_x] \\ & + U^{-3}[64 \sum_{<xy>:|x-y|=\sqrt{2}} V_x V_y + 16 \sum_{<xy>:|x-y|=2} V_x V_y - 16 \sum_x V_x + \sum_{X \in E_4} c_{4,X} V_X] \end{aligned}$$

E_4 is the collections of sets X which appear at fourth order and contain a pair of sites x, y with $|x-y| = 1$. There are only a few such sets and we can compute their coefficients explicitly, but as we will see their actual values play no role in the proof. If $X \in E_4$ and $V_X \neq 0$, then there is a nearest neighbor pair x, y with $V_x V_y = 1$. This gives a contribution of $8U^{-1}$ to H_4 which is much larger than the order U^{-3} contribution from $c_{4,X} V_X$.

It was shown in [5] that for configurations with density between 1/5 and 1/4 which minimize H_4 every 3 by 3 block of sites must look like one of the four configurations shown in figure 2 . (We will include a proof of this later.) Watson [8] made the following observation that will play an essential role in our proof.

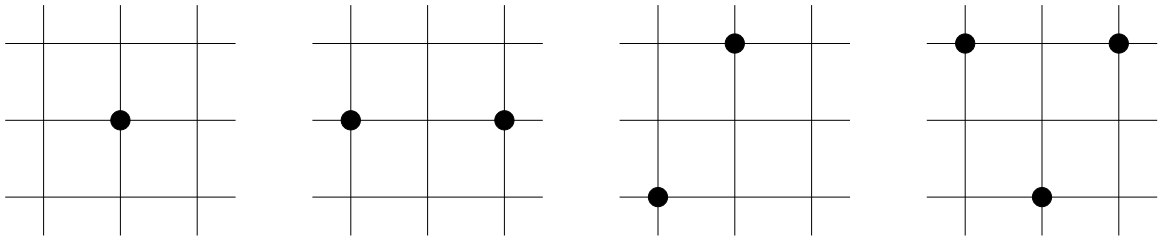

Figure 2 : For densities between 1/5 and 1/4, fourth order perturbation theory implies that in a ground state every 3 by 3 square must be one of the above cases, up to lattice symmetries.

Lemma 1 *If every 3 by 3 block equals one of those shown in figure 2 (up to a lattice symmetry), then the configuration corresponds to a tiling of the lattice by squares and diamonds in which every vertex looks like one of the four types shown in figure 3 up to a lattice symmetry.*

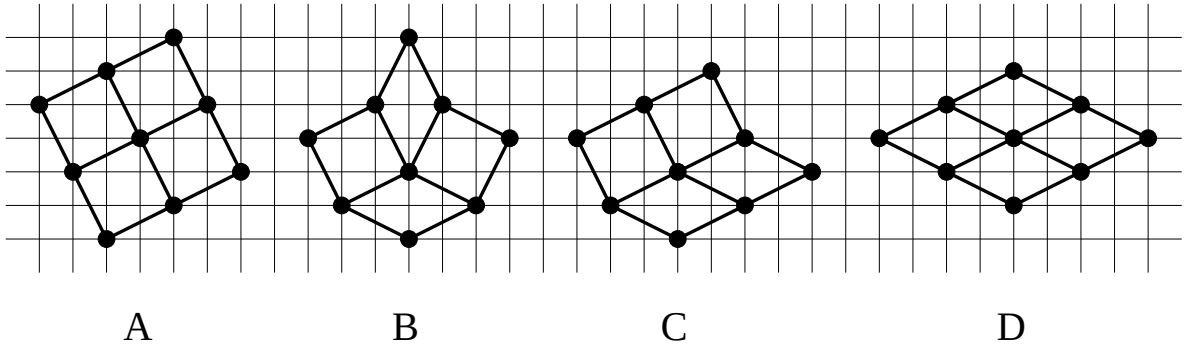

Figure 3 : For densities between 1/5 and 1/4, every ground state corresponds to a tiling of the plane by squares and diamonds in which every vertex must be one of the four types shown above. The ions at the center of each of these figures are called type A, B, C or D ions, respectively.

Proof [8]: Note that the 3 by 3 blocks we are using can overlap. Thus the condition that every one of these blocks is one of those shown in figure 2 puts many constraints on the configuration. We start with a site at which there is an ion. Using the fact that every 3 by 3 block is one of those shown in figure 2 we work outwards from the initial ion and determine all possible configurations in the neighborhood of the inital ion. We find that the configuration must look like one of the four cases shown in figure 3 . ∎

It is important to note that the proof of the lemma is local. If we have a configuration in which some 3 by 3 blocks are not one of those shown in figure 2 , then we can still conclude that in the parts of the lattice where the 3 by 3 blocks are one of those shown in the figure the configuration must be given by a square-diamond tiling. We will say that an ion is type A, B, C or D if the configuration in the neighborhood of the ion agrees with that shown in figure 3 up to a lattice symmetry. Note that in regions where the configuration does not correspond to a square-diamond tiling there will be ions that are not any of these four types.

The tenth order Hamiltonian H_{10} contains too many terms to list here. However, we can organize the Hamiltonian so that we only need the actual values of the coefficients of a modest number of them. The values of the coefficients of the terms in H_{10} are important only in regions where H_4 is minimized. By the lemma the configuration corresponds to a square-diamond tiling in such regions. In these tilings two ions cannot be separated by a distance $1, \sqrt{2}, \sqrt{8}$ or 3. So we define E_{10} to be the collection of sets that appear at tenth order or lower and contain a pair of sites x, y with $|x-y|^2$ equal to $1, 2, 8$ or 9. For $X \notin E_{10}$ the coefficients $c_{6,X}, c_{8,X}, c_{10,X}$ are given in table 1.

term	6th	8th	10th	A	B	C	D
(0,0)	64	112	-704	1	1	1	1
(0,0), (2,0)	96	-1360	-1440	0	1/2	1/2	1
(0,0), (2,1)	216	-768	-14000	2	2	2	2
(0,0), (3,1)		512	640	2	1	1	0
(0,0), (4,0)		32	1120	0	1/2	1/2	2
(0,0), (3,2)			4000	0	0	1/2	2
(0,0), (4,1)			1000	0	2	1	0
(0,0), (5,0)			40	2	0	1/2	0
(0,0), (2,0), (1,2)		-2592	10560	0	1	1	2
(0,0), (2,0), (4,0)		192	1760	0	0	0	1
(0,0), (2,0), (1,3)			-7040	0	0	0	0
(0,0), (2,0), (3,2)			-5280	0	0	1	4
(0,0), (2,1), (4,0)			-3960	0	1	1	2
(0,0), (2,1), (4,1)			1320	0	2	1	0
(0,0), (2,1), (-1,2)			-15840	4	2	2	0
(0,0), (1,2), (2,0), (3,2)			15840	0	0	1/2	2

Table 1 : The sixth, eighth and tenth order terms in the Hamiltonian when restricted to configurations that correspond to tilings by squares and diamonds.

Now we are ready to state and prove the main inequalities that will show there is phase separation for densities between 1/5 and 1/4 other than 2/9.

Theorem 2 *Let M be the number of 3 by 3 blocks in which the configuration is not one of those shown in figure 2 . Let n_A, n_B, n_C and n_D be the number of type A, B, C and D ions respectively (figure 3). Consider an L by L lattice so there are L^2 sites, and let ρ be the ion density so there are ρL^2 ions. Then there are polynomials $p_1, p_2, \cdots, p_6$ in U^{-1} and functions f_1, f_2, f_3, f_4 of U^{-1} such that*

$$\frac{16}{3}U^{-3}M \leq H_4 - p_1\rho L^2 - p_2 L^2 = O(U^{-1})M \tag{7}$$

$$H_{10} - p_3\rho L^2 - p_4 L^2 = 224U^{-7}n_D + 2340U^{-9}n_C + 12240U^{-9}n_D + O(U^{-5})M \tag{8}$$

$$H_{10} - p_5\rho L^2 - p_6 L^2 = 224U^{-7}n_A + 2340U^{-9}n_C + 12240U^{-9}n_A + O(U^{-5})M \tag{9}$$

$$H_\infty - f_1\rho L^2 - f_2 L^2 = O(U^{-11})(n_C + n_D + M) \tag{10}$$

$$H_\infty - f_3\rho L^2 - f_4 L^2 = O(U^{-11})(n_A + n_C + M) \tag{11}$$

$O(U^{-k})$ denotes a quantity whose absolute value may be bounded by a constant times U^{-k}.

Proof: The inequality for H_4 was proved in [5]. We include a short proof for completeness. Let B be a 3 by 3 block of sites. (So it contains 9 sites.) Let z be the center of B. Define

$$\begin{aligned} H_B \quad &= U^{-1}\frac{4}{3}\sum_{<xy>\subset B:|x-y|=1} V_x V_y + U^{-3}[16\sum_{<xy>\subset B:|x-y|=\sqrt{2}} V_x V_y + \frac{16}{3}\sum_{<xy>\subset B:|x-y|=2} V_x V_y \\ &-16V_z - \frac{32}{3}\sum_{x\in B:|x-z|=1} V_x - \frac{16}{3}\sum_{x\in B:|x-z|=\sqrt{2}} V_x + 16 + \sum_{X\subset B, X\in E_4}\frac{c_{4,X}\,V_X}{m_X}] \end{aligned}$$

where m_X is the number of translates of X that are contained in B. Now consider $\sum_B H_B$ where the sum is over all 3 by 3 blocks. (So some of them overlap.) A pair $< xy >$ with $|x-y| = 1$ is contained in 6 different blocks, a pair with $|x-y| = \sqrt{2}$ in 4 different blocks, and a pair with $|x-y| = 2$ in 3 different blocks. Using these facts we find

$$\sum_B H_B = H_4 + (16U^{-1} - 64U^{-3})\rho L^2 + 16U^{-3}L^2 \tag{12}$$

So to complete the proof we must show that H_B vanishes if B is one of the blocks shown in figure 2 and is at least $\frac{16}{3}U^{-3}$ otherwise. First note that if the block contains a pair of nearest neighbor ions then the second order part of H_4 is at least $\frac{4}{3}U^{-1}$. Since the fourth order part is smaller by a factor of U^{-2}, this shows that $H_B \geq \frac{16}{3}U^{-3}$ for all such configurations if U is large enough. Now suppose that the block does not contain any nearest neighbor ions. Note that this implies that $V_X = 0$ for all $X \in E_4$. So we can easily compute H_B for such configurations. We find that for all 3 by 3 blocks that do not contain a nearest neighbor pair of ions and which are not in figure 2 , H_B is at least $\frac{16}{3}U^{-3}$. H_B vanishes on the configurations in figure 2 . This completes the proof of (7).

To prove (8) and (9) we first consider configurations which correspond to a square-diamond tiling. If $X \in E_{10}$ then $V_X = 0$ in these configurations. We will consider two X's to be equivalent if they are related by a translation, reflection and or rotation. For $X \notin E_{10}$ there are 16 equivalence classes, listed in table 1. For each equivalence class we want to write the number of X in the class with $V_X = 1$ in terms of n_A, n_B, n_C, n_D. Consider the second equivalence class. It contains those X's of the form $X = \{x, y\}$ with $|x - y| = 2$. The number of such X with $V_X \neq 0$ in figure 3 is 0,2,2, or 4 for A,B,C, or D, respectively. However, this overcounts the number of X with $V_X \neq 0$. Each X is counted 4 times. So the number of X's in the second equivalence class with $V_X = 1$ is $0n_A + \frac{1}{2}n_B + \frac{1}{2}n_C + n_D$. These coefficients $0, \frac{1}{2}, \frac{1}{2}, 1$ along with the coefficients for all the other equivalence classes are given in table 1. We should emphasize that the overcounting factor is not always 4. It varies from equivalence class to equivalence class, and in one case within the equivalence class. Using table 1 we find that for configurations which correspond to a square-diamond tiling,

$$\begin{aligned} H_{10} \quad &= U^{-5}(496n_A + 544n_B + 544n_C + 592n_D) \\ &+U^{-7}(-400n_A - 4168n_B - 4168n_C - 7712n_D) \\ &+U^{-9}(-90704n_A - 48664n_B - 46324n_C + 5616n_D) \end{aligned}$$

The quantities n_A, n_B, n_C and n_D are not all independent. Each ion corresponds to a vertex in the square-diamond tiling, so

$$n_A + n_B + n_C + n_D = \rho L^2 \tag{13}$$

By considering the areas associated with each of the four types of vertices in figure 3 , we see that

$$5n_A + \frac{9}{2}n_B + \frac{9}{2}n_C + 4n_D = L^2 \tag{14}$$

Using these two equations we can eliminate n_A and n_B from our expression for H_{10}. The result is (8). If we use the two equations to eliminate n_B and n_D, then the result is (9).

This proves (8) and (9) for configurations that correspond to a square-diamond tiling. Now consider a configuration that does not. The number of sites in the region where it does not correspond to such a tiling is at most $9M$. Thus the terms in H_{10} that intersect this region can contribute at most $O(U^{-5})M$. Outside of this region we can apply the above argument. There will be errors at the boundary of the region in which there is a square-diamond tiling since there will be incomplete squares and diamonds, but the contribution of these errors is also $O(U^{-5})M$. Equations (13) and (14) are not true for a general configuration, but the difference between the right and left side of these equations is bounded by a constant times M. This completes the proof of (8) and (9).

Finally, we must prove (10) and (11). We only give the proof of (10). A similar argument proves (11), or it may be obtained from (10) by showing $|n_A - n_D - 2L^2 +$

$9\rho L^2|$ is bounded by a constant times M. To compare a term $c_{2m,X}V_X$ in H_∞ with the corresponding term for the configurations in figure 1 , we need to know if X is contained in a region where the configuration agrees with one of the configurations in figure 1 . So we make the following definitions. For a lattice site x and positive integer r, let $B_r(x)$ be the set of sites such that the l^1 distance from x to y is at most r. Given a configuration, let A_m be the set of sites with a type A ion such that $B_m(x)$ is a subset of configuration A in figure 1 . B_m is defined analogously using configuration B. Define $\hat{h}_{2m,X} = h_{2m,X}/|X|$ so that

$$H_\infty = \sum_{m=6}^{\infty} U^{-2m+1} \sum_x \sum_{X:x\in X} \hat{h}_{2m,X} V_X \tag{15}$$

Since $V_X = 0$ if $V_x = 0$, we can restrict the sum over x to sites with an ion.

Let I denote the sites with an ion. We start by comparing H_∞ with the sum over a subset of the terms in H_∞:

$$|H_\infty - \sum_{m=6}^{\infty} U^{-2m+1} \sum_{x\in A_m\cup B_m} \sum_{X:x\in X} \hat{h}_{2m,X} V_X| = |\sum_{m=6}^{\infty} U^{-2m+1} \sum_{x\in I\setminus(A_m\cup B_m)} \sum_{X:x\in X} \hat{h}_{2m,X} V_X|$$

$$\leq \sum_{m=6}^{\infty} U^{-2m+1} |I \setminus (A_m \cup B_m)| c^m \tag{16}$$

using (4). We need to estimate the size of $I \setminus (A_m \cup B_m)$. Let $x \in I \setminus (A_m \cup B_m)$. Then $B_m(x)$ is not a subset of configuration A or B in figure 1 . So either (i) $B_m(x)$ is not a subset of any square-diamond tiling, (ii) $B_m(x)$ is a subset of a square-diamond tiling which contains a type C or type D vertex, or (iii) $B_m(x)$ is a subset of a square-diamond tiling which contains both type A and type B vertices. In case (i) $B_m(x)$ must intersect a 3 by 3 block that is not one of those in figure 2 . Note that it is not possible for a tiling to contain both type A and type B vertices, but no type C or D, so case (iii) never happens. Thus we can associate with each site in $I \setminus (A_m \cup B_m)$ either a "bad" 3 by 3 block or a type C or type D vertex. The number of sites that are associated with the same 3 by 3 block or type C or type D vertex is bounded by dm^2 for some constant d. Thus

$$|I \setminus (A_m \cup B_m)| \leq dm^2(n_C + n_D + M) \tag{17}$$

Thus (16) is

$$\leq \sum_{m=6}^{\infty} U^{-2m+1} c^m dm^2 (n_C + n_D + M) = O(U^{-11})(n_C + n_D + M) \tag{18}$$

Let e_A be the energy per site from H_∞ when the entire finite lattice contains configuration A in figure 1 , and let e_B be the same quantity for configuration B in figure 1 . Let

$$5e_A = \sum_{m=6}^{\infty} U^{-2m+1} a_{2m} \tag{19}$$

If $x \in A_m$ then the definition of A_m implies that

$$\sum_{X:x\in X} \hat{h}_{2m,X} V_X = a_{2m} \tag{20}$$

Thus

$$|\sum_{m=6}^{\infty} U^{-2m+1} \sum_{x\in A_m} \sum_{X:x\in X} \hat{h}_{2m,X} V_X - 5n_A e_A| \leq \sum_{m=6}^{\infty} U^{-2m+1} \sum_{x\in A\setminus A_m} |a_{2m}| \tag{21}$$

Since $A \setminus A_m \subset I \setminus (A_m \cup B_M)$, (17) implies $|A \setminus A_m| \leq cm^2(n_C + n_D + M)$. This shows that (21) is $O(U^{-11})(n_C + n_D + M)$.

A similar argument shows

$$|\sum_{m=6}^{\infty} U^{-2m+1} \sum_{x\in B_m} \sum_{X:x\in X} \hat{h}_{2m,X} V_X - \frac{9}{2} e_B n_B| = O(U^{-11})(n_C + n_D + M) \tag{22}$$

Combining our bounds on (16) and (21) with (22) shows

$$|H_\infty - 5e_A n_A - \frac{9}{2} e_B n_B| = O(U^{-11})(n_C + n_D + M) \tag{23}$$

which proves (10). ∎

The main theorem follows easily from the inequalities we have proved by a "variational" argument.

Proof of theorem 1: First we prove the statement about the ground state for density 2/9. Configuration B has $M = 0$ and only type B vertices, so theorem 2 immediately implies it is a ground state. Any other ground state must have $M = 0$ and no type C or D vertices. The condition $M = 0$ implies the configuration is a square diamond tiling. The only tiling which contains only A and B vertices and has density 2/9 is configuration B in figure 1 .

Now we turn to the proof of the statements for densities between 1/4 and 1/5. We will construct a trial configuration with relatively low energy and then use the inequalities in theorem 2 to prove theorem 1. We give the proof for the case of densities in $(1/5, 2/9)$. The proof for densities in $(2/9, 1/4)$ is similar.

Divide the L by L square into two rectangles and put configuration A in figure 1 on one side and configuration B on the other side. The relative areas of the two rectangles are chosen to give the desired density. The number of 3 by 3 blocks which do not agree with one of those in figure 2 is bounded by a constant times L. Thus $H_4 - p_1\rho L^2 - p_2 L^2$ is $O(U^{-1})L$. n_C and n_D are both zero, so $H_{10} - p_3\rho L^2 - p_4 L^2$ is $O(U^{-5})L$ and $H_\infty - f_1\rho L^2 - f_2 L^2$ is $O(U^{-11})L$. Any ground state must have energy no greater than that of our trial configuration, so theorem 2 implies that in a ground state

$$\frac{16}{3}U^{-3}M + 224U^{-7}n_D + 2340U^{-9}n_C + 12240U^{-9}n_D + O(U^{-5})M$$
$$+O(U^{-11})(n_C + n_D + M) \leq O(U^{-1})L$$

which may be rearranged as

$$[\frac{16}{3}U^{-3} + O(U^{-5}) + O(U^{-11})]M + [224U^{-7} + 12240U^{-9} + O(U^{-11})]n_D$$
$$+[2340U^{-9} + O(U^{-11})]n_C \leq O(U^{-1})L$$

If U is large enough this implies that $M + n_C + n_D$ is bounded by a constant times $U^8 L$. Now take Λ_0 to be the union of all the 3 by 3 blocks which do not agree with one of the configurations in figure 2 together with the union over all type C and type D ions of the region associated with the ion shown in figure 3 . In $\Lambda \setminus \Lambda_0$ the configuration must be a square diamond tiling with no C or D vertices. Note that type A and type B vertices cannot be adjacent in the tiling, i.e., separated by a distance $\sqrt{5}$. However, this does not quite insure that each component contains only type A or type B vertices. For example one can have a component that consists of two large regions which are connected only by a single line of sites. Then one can have type A vertices on one side of the narrow connection and type B on the other side. To eliminate this, redefine Λ_0 to be the original Λ_0 plus all sites within a distance d of the original set. If d is chosen large enough we eliminate the above problem and every connected component of $\Lambda \setminus \Lambda_0$ will be a square-diamond tiling with only type A or type B vertices. ∎

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